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We show that the Ricatti form of the Schroedinger equation can be reformulated in terms of two linear equations depending on an arbitrary function G. When G and the potential are polynomials, the solutions of these two equations are entire functions (L and K) and the zeroes of K are identical to those of the wave function. Requiring such a zero at a large but finite value of the argument yields the low energy eigenstates with exponentially small errors. Judicious choice of G can improve dramatically the numerical treatment. The method yields many significant digits with modest computer means.

PACS: 03.65.Ge, 03.65.-w, 02.30.Em, 02.30.Mv, 10.10.St, 33.20.-t

I. INTRODUCTION

Quantum anharmonic oscillators appear in a wide variety of problems in molecular, nuclear or condensed matter physics. Typically, anharmonic terms appear in expansions about a minimum of a potential, when ones tries to incorporate the non-linear features of the forces responsible for this equilibrium. The most celebrated example is the quartic anharmonic oscillator [1] where a λx^4 term is added to the usual harmonic Hamiltonian. Introducing bilinear couplings among a set of such oscillators leads to a rich spectrum, for instance, multiphonon bound states in one-dimensional lattice models [2]. More generally, one can think about the $\lambda\phi^4$ (or higher powers of ϕ) field theories in various dimensions as systems of coupled anharmonic oscillators.

Anharmonic terms can be treated perturbatively and the perturbative series can be represented by Feynman diagrams. Unfortunately, the coefficients of the series [1,3] have a factorial growth and the numerical values obtained from the truncated series have an accuracy which is subject to limitations. At fixed coupling, there is an order at which an optimal accuracy is reached. At fixed order, there is a value of the coupling beyond which the numerical values are meaningless even as an order of magnitude. In the case of the single-well quartic potential, Padé approximants can be used for the series or its Borel transform. Rigorous proofs of convergence can be established in particular cases [4]. Unfortunately, such a method does not apply to the case of the double-well potential [5] where instanton effects [6,7] need to be taken into account. It should also be noted that even when Padé approximants converge, the convergence rate may be slow. Strong coupling expansions [8] or variational interpolations [9] sometimes provide more accurate results.

The above discussion shows that finding an expansion which can be used *indiscriminately* for most quantum mechanical problems with polynomial potentials remains a challenging problem. In this article, we describe a numerical method which achieves this goal and can be used as a starting point for an analytical treatment. The basic elements of this numerical method were sketched in Ref. [10] and applied to the quartic anharmonic oscillator. The values of the first ten eigenvalues with 30 significant digits provided for a particular coupling, have been used to test new theoretical methods [11]. However, important questions were left open in Ref. [10]. The main goal of this article is to propose a new formulation in which these open questions have straightforward answers and a general procedure can be made available to a large number of potential users.

The present paper is intended for a broad audience. On one hand, one can use the results presented here as a "recipe" to find the energy levels of complicated polynomial potentials. This task can be done by finding the zeroes of a function defined below in Eq. (8) and which can be constructed with a short computer program. Alternatively, the method can be used to determine the coefficients of a phenomenological potential using an experimental spectrum. On the other hand, our article addresses theoretical questions such as the role played by the large field configurations in the path-integral. In order to let the reader decide what parts of the paper are relevant for a particular need, we first give a brief summary of the results presented before entering in technical details.

II. AN OVERVIEW OF THE NEW RESULTS PRESENTED

The basic observation of Ref. [10], is that an accurate description of the behavior of the wave function at large values of its argument x can be used to capture the sensitive dependence of this behavior on the value of the energy eigenvalue E and set sharp bounds on E using the normalizability condition. The accurate description was obtained by noticing that the solution of the associated Ricatti equation for the logarithmic derivative of the wave function can be represented as a ratio (L/K) of *entire* functions. As explained in Ref. [10] and in Section V below, high accuracy estimates of the energy levels can be obtained by solving $K(x_{max}) = 0$ for E using a polynomial approximation of K valid near x_{max}. It should

be noted that $K(x_{max})$ is also a polynomial in the anharmonic couplings and consequently one can also construct sets of equations for these couplings given some values of the energy levels.

Despite the fact that one can easily obtain hundred of correct significant digits with this procedure, several important questions were left open in [10]. Actually, our original intent was not to calculate energy levels but to construct the creation operator for the anharmonic oscillator. The matrix elements of this operator can be expressed in terms of functions L and K that we realized could also be used to construct solutions of the Ricatti equation. Both functions were dependent on a quantity (which was denoted Δ) representing the difference between two subsequent energy levels. However, the ratio L/K was found to be independent of Δ, order by order in an expansion in Δ about 0. We did not understand this invariance but realized that it could be exploited to optimize the numerical treatment.

Three issues related to this invariance needed to be settled. First, one would like to have a general explanation regarding the origin of the invariance and to understand how it affects the numerical stability of the solutions of $K(x_{max}) = 0$. Second, the use of the method for parity non-invariant potentials appeared to be unduly complicated [12]. Third, spurious (Δ-dependent) zeroes in K were found and inappropriate choices of Δ can prevent automatized calculations of spectra.

We present here a new formulation of the problem where these questions can be answered. In this new formulation, the two basic linear equations are first order instead of second order (as in [10]). In the new formulation, these equations depend on an arbitrary *function* denoted $G(x)$. This freedom can be interpreted as a local gauge invariance. The wave function is invariant under the local gauge transformations. The new equations are presented in Section III, where we also explain that the basic equations of Ref. [10] are the derivative of the ones presented here in a particular family of gauges indexed by Δ. We will show that if G is a polynomial, there are no spurious zeroes of K. In the following, unless specified otherwise, G will be assumed to be polynomial.

In section IV, we show how to construct power series for L and K. The complications in the case of parity non-invariant potentials (such as asymmetric double-wells) are minimal. These series define *entire* functions for arbitrary polynomial potentials. By using truncations at a given order, we obtain accurate representations of the logarithmic derivative of the wave function within a certain range of x which depends on the order of truncation and the details of the potential. This can be used to identify bifurcations in the asymptotic behavior of the solution as we change the value of E. This is explained in Section V for a general potential (not necessarily parity invariant). Section V also provides a qualitative picture of the quantization condition in terms of the general properties of the flows of the Ricatti equation. We hope that this simple picture will some day find its way to introductory quantum mechanics textbooks. It translates into a practical recipe, namely finding the values of E for which $K(x_{max}) = 0$.

It should be noted that in the past, Padé approximants have been used in conjunction with the Ricatti equation [13]. The quantization condition used in Ref. [13] was that the approximants give one additional coefficient in the Taylor expansion. This procedure depends only on the coefficients of the expansions used and there is no reference to any particular value of x (as our x_{max}). Consequently, there is no obvious connection between the two approaches.

In the next two sections, we show how to turn the gauge invariance to our advantage. In Section VI, the quantitative aspects of the bifurcation are discussed with an exponential parametrization similar to the one used to determine Lyapounov exponents in the study of chaotic dynamical system. We show that the exponents are G-dependent. In Section VII, we show in a particular example that for an expansion at a given order, a judicious choice of gauge can improve tremendously the numerical accuracy of an energy level. We give an intuitive explanation of the two principles which allow to make the optimal choice.

From Eq. (7), one can reinterpret the condition $K(x_{max}) = 0$ as coming from a slightly different problem where the potential becomes infinite at x_{max}. If the potential is large at x_{max} this has little influence on the low energy spectrum. The goal of Section VIII is to make this statement quantitative, namely, determine how the error depends on x_{max} and V. In the path-integral formulation, the fact that the potential becomes infinite at x_{max} means that paths with values of x larger than x_{max} are not taken into account. It has been argued [14,15] that these configurations are responsible for the asymptotic behavior of the regular perturbative series. In Ref. [15], we showed that the perturbative series of the modified problem were convergent. The error formula sets the accuracy limitations of this approach.

Finally, an anharmonic oscillator can be considered as a field theory with one time and zero space dimensions. It can be used to test approximate methods such as perturbative expansions or semi-classical procedures. An illustrative example is given in Ref. [19] where multi-instanton effects were considered and where the splitting of the two lowest levels of a double-well problem were estimated with more than hundred digits. In Section IX, we show that our method can be used to reproduce all these digits. In the future, we plan to test semi-classical methods for asymmetric wells [6,7] which are often used in cosmological context.

In summary, the main advantages of the method presented here are its great generality and the systematic control of the errors.

III. BASIC EQUATIONS AND THEIR GAUGE-INVARIANCE

We consider a one-dimensional, time-independent Schroedinger equation $H\Psi = E\Psi$, for an Hamiltonian

$$H = \frac{p^2}{2m} + \sum_{l=1}^{2l} V_j x^j \ . \tag{1}$$

As well-known, one can reexpress the wave function in terms of its logarithmic derivative

$$\Psi(x) \propto \mathrm{e}^{-\frac{1}{\hbar}\int_{x_0}^{x} dy\phi(y)} \ , \tag{2}$$

and obtain the Ricatti form of the equation:

$$\hbar\phi' = \phi^2 + 2m(E-V) \ . \tag{3}$$

It is assumed that $m > 0$ and that the leading power of V is even with a positive coefficient ($V_{2l} > 0$).

Writing $\phi = L/K$, we obtain a solution of Eq. (3) provided that we solve the system of equations:

$$\hbar L' + 2m(V-E)K + GL = 0 \tag{4}$$
$$\hbar K' + L + GK = 0 \tag{5}$$

where $G(x)$ is an unspecified function. This can be seen by multiplying (4) by K, (5) by L and eliminating GKL by taking the difference. One then obtains the Ricatti equation (3) multiplied by K^2. Near a zero of K, one can check that Eqs. (4-5) remain valid, namely they impose that ϕ has a simple pole with residue $-\hbar$. This allows the wave function to change sign as the contour goes around the pole on either side. This also means that there is a one-to-one correspondence between the zeroes of Ψ and the poles of ϕ.

Eqs. (4-5) are invariant under the *local* transformation

$$\begin{aligned} L(x) &\to Q(x)L(x) \\ K(x) &\to Q(x)K(x) \\ G(x) &\to G(x) - \hbar Q'(x)/Q(x) \ , \end{aligned} \tag{6}$$

where $Q(x)$ is an arbitrary function. It is clear that this transformation leaves ϕ and the wave function unchanged. If we choose $G = 0$ and eliminate L using Eq. (5), we recover the Schroedinger equation for K. Starting from this gauge and making an arbitrary transformation, we find that in general

$$K(x) \propto \Psi(x)\mathrm{e}^{-\frac{1}{\hbar}\int_{x_0}^{x} dyG(y)} \tag{7}$$

This shows that when G is polynomial, K is simply Ψ multiplied by an entire function *with no zeroes* [16]. This means that the zeroes of K and Ψ are identical. In other words, there are no spurious zeroes when G is polynomial.

By taking the derivative of Eqs. (4) and (5) and choosing $G(x)$ appropriately, one can obtain the basic Equations used in [10]. The explicit form of $G(x)$ is reached by comparing the two sets of equations and integrating one of the differences. The two possibilities are compatible. The resulting integral expression can be worked out easily by the interested reader. The only important point is that the G found that way is in general not polynomial, justifying the spurious zeroes found with the original formulation.

IV. SOLUTIONS IN TERMS OF ENTIRE FUNCTIONS

The function G can be chosen at our convenience. For instance, we could impose the condition $K = 1$ by taking $G = -L$ and recover the Ricatti equation for L. However, the main advantage of Eqs. (4-5) is that they are linear first order differential equations with variables coefficients. It is well-known [17] that if we consider these equations for complex x, the solutions inherit the domain of analyticity of the coefficients (provided that this domain is simply connected). If the coefficients are entire functions, there exists a unique entire solution corresponding to a particular set of initial values. In the following, we restrict ourselves to the case where V and G are polynomials.

One can construct the unique solution corresponding to a particular choice of initial values $L(0)$ and $K(0)$ by series expansions. Using $K(x) = \sum_{n=0}^{\infty} K_n x^n$ and similar notations for the other functions, one obtains the simple recursion

$$\begin{aligned} L_{n+1} &= \frac{-1}{\hbar(n+1)}\Big(\sum_{l+p=n}(2mV_lK_p + L_lG_p) - 2mEK_n\Big) \\ K_{n+1} &= \frac{-1}{\hbar(n+1)}\Big(L_n + \sum_{l+p=n} K_lG_p\Big) \end{aligned} \tag{8}$$

Given L_0 and K_0, these equations allow to determine all the other coefficients. For potentials which are parity invariant, and if G is an odd function, L and K can be assigned definite and opposite parities. In this case, we can impose the initial conditions $K_0 = 1$ and $L_0 = 0$ for even wave functions and $K_0 = 0$ and $L_0 = 1$ for odd wave functions. If the Hamiltonian has no special symmetry, as for instance in the case of an asymmetric double-well, one could leave L_0 indeterminate and fix it at the same time as E using conditions on the wave function or its derivative at two different points. These two conditions translate (in good approximation) into two polynomial equations in L_0 and E and can be solved by Newton's method.

The fact that Eqs. (8) determines entire functions provided that V and G are polynomials can be inferred directly from the fact that the coefficients will decrease as $(n!)^{-\kappa}$ for some positive power κ to be determined and in general depending on the choice of G. If the leading

term in V is $V_{2l}x^{2l}$, one expects from Eq. (3) that for x large enough,

$$\phi(x) \simeq \pm\sqrt{2mV_{2l}}x^l \ , \tag{9}$$

and asymptotically,

$$\Psi(x) \propto \mathrm{e}^{-\frac{\pm 1}{(l+1)\hbar}\sqrt{2mV_{2l}}x^{l+1}} \ . \tag{10}$$

Looking at the general expression for K given in Eq. (7), one sees that K will have the same asymptotic behavior provided that the integral of G grows not faster than x^{l+1}. If this is the case, then $\kappa = 1/(l+1)$. This behavior is well observed in empirical series.

Note that if G grows faster than x^l, the coefficients decay more slowly and the procedure seem to be less efficient. In the following, we will mostly discuss the case $l = 2$. If we require that G is an odd polynomial growing not faster than x^2, this means that G is homogeneous of degree 1.

V. QUANTIZATION FROM GLOBAL FLOW PROPERTIES

We now consider the solutions of Eq. (3) obtained by varying E with fixed initial values. It is convenient to introduce an additional parameter s and to rewrite the original equation as a 2-dimensional ODE with a s-independent r.h.s .

$$\hbar\dot{\phi} = \phi^2 + 2m(E - V(x)) \tag{11}$$

$$\dot{x} = 1 \ , \tag{12}$$

where the dot denotes the derivative with respect to s.

The flows in the (x, ϕ) plane have some simple global properties that we now proceed to describe. We consider a solution (phase curve) with initial condition $x = x_0$ and $\phi = \phi_0$ at $s = 0$. We assume that for these values the r.h.s of Eq. (11) is > 0. It will become clear later that if such a choice is impossible, a normalizable wave function cannot be constructed. With this assumption, the phase curve starts moving up and right as s increases, possibly going through simple poles with residues $-h$. This situation persists unless the r.h.s. of (11) becomes zero. We call the separating curves defined by a zero for the r.h.s of Eq. (11), $\phi = \pm\sqrt{2m(V(x) - E)}$, "$WKB$ curves". After a phase curve crosses (horizontally) a WKB curve, it moves right and down. If it crosses the WKB curve again, we can repeat the discussion as at the beginning.

If we compare two phase curves with identical initial conditions but different E, the one with larger E initially lays above the other one. If the one with lower E has a first pole at x_1, then the one with larger E has a first pole at some $x < x_1$. Remembering that the poles of ϕ are the zeroes of Ψ, this rephrases the main idea behind the Sturm-Liouville theorem.

The above discussion is valid for any E. We would like to know which choices of E lead to a normalizable wave function. For x large enough, we have the two possible approximate behaviors given by Eq. (9). Given the sign convention of Eq. (2), only the positive asymptotic solution leads to a normalizable wave function. For x large enough, Eq. (2) also provides a good approximation of the upper and lower part of the "last" WKB curve (i.e., the foremost right). In addition we assume that x is large enough so that the upper (lower) part of the WKB curve increases (decreases) monotonically. For such values of x, if a phase curve crosses the WKB curve, it will do so horizontally and move *inside* the region where the r.h.s. of Eq. (11) is negative. In other words, this region is a sink. When the phase curve enters this region, ϕ decreases and the phase curve approaches the lower part of the WKB curve. In this case, the wave function is not normalizable.

An exact energy eigenstate E_n is obtained when the wave function has its last zero at infinity. When E is fine-tuned to that value, ϕ follows closely the upper branch of the WKB curve. This trajectory in unstable under small changes in E. If the energy is slightly increased with respect to E_n, ϕ develops a pole and reappears on the lower part of the WKB curve. If the energy is slightly decreased with respect to E_n, ϕ crosses the upper part of the WKB curve and reaches the lower part of the WKB curve. This sensitive dependence on E can be exploited to obtain sharp upper and lower bounds on E_n [10]. This is illustrated in Fig. 1 in the case of the ground state of the quartic single-well anharmonic oscillator with $m = 1/2$, $\hbar = 1, V_2 = 1$ and $V_4 = 0.1$. All the figures in this section and the next two sections have been done with this particular example.

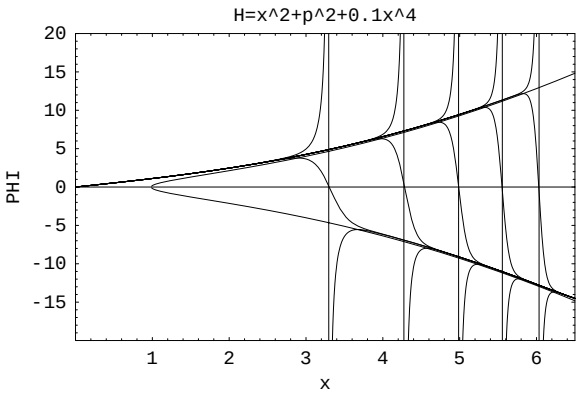

FIG. 1. Bifurcations of $\phi(x)$ from the upper part of the WKB curve associated with the ground state energy E_0 for energies $E_0 \pm 10^{-5}$, $E_0 \pm 10^{-10}$, $E_0 \pm 10^{-15}$, $E_0 \pm 10^{-20}$ and $E_0 \pm 10^{-25}$ (from left to right).

The above discussion shows that one can obtain sharp upper bounds on an energy level by showing that it corresponds to a zero of Ψ for some large positive value of x that we will denote x_{max}. In other words, we consider a slightly different problem where the potential becomes infinite at x_{max}. We will see in Section VIII that the

error associated with this modification can be made exponentially small.

We are now in position to discuss the initial value ϕ_0. For parity invariant potentials, one only needs to consider the cases $\phi_0 = 0$ (even Ψ) or $\phi_0 = -\infty$ (odd Ψ) at $x_0 = 0$. For potentials with no reflection symmetry, one needs to insure that the appropriate behavior is reached when $x \to -\infty$. This can be implemented in good approximation by requiring that the wave function has also a zero at some large negative value x_{min}. For potentials with a reflection symmetry about another point x_1 than the origin, one can impose that the wave function ($K(x_1) = 0$) or its derivative ($L(x_1) = 0$) vanish at that point. In all cases, we have an independent condition which allows to determine ϕ_0.

The sensitive dependence on E is also present in the asymptotic behavior of K. If the energy is slightly increased with respect to E_n, K reaches zero at a finite value of x. If the energy is slightly decreased with respect to E_n, K increases rapidly. This is illustrated in Fig. 2 for the same example as in Fig. 1.

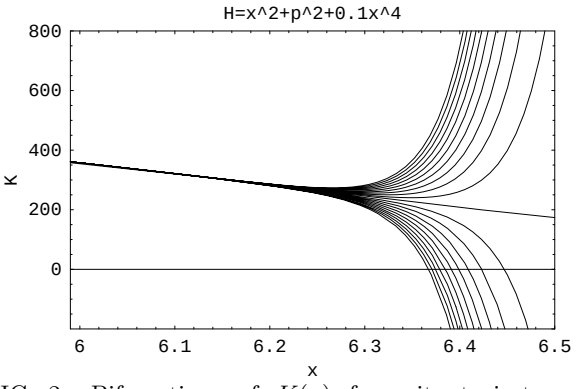

FIG. 2. Bifurcations of $K(x)$ from its trajectory for $E = E_0$. The changes in E are $\pm 10^{-30}$, $\pm 2 \times 10^{-30}, \ldots,$ $\pm 10^{-29}$

In summary, the condition

$$K(x_{max}) = 0 \tag{13}$$

provides sharp upper bound on the energy levels. The lower part of Fig. 2 makes clear that as x_{max} increases, sharper bounds are reached. For potential that are not parity invariant, an additional condition has to be imposed. In all cases, one obtains polynomial equations which can be solved for the energy levels given the potential or vice-versa using Newton's method.

VI. G-DEPENDENCE OF THE BIFURCATION

The bifurcation in K can be approximately characterized by local exponents. If we consider the departure $\delta K(x)$ from $K(x)$ calculated at some energy level E_n, we have the approximate behavior:

$$\delta K(x) \simeq C(E - E_n)\mathrm{e}^{xB} \ . \tag{14}$$

In other words $\ln(|\delta K(x)|)$ is linear with a slope B independent of the choice of E and an intercept that varies like $\ln(|E - E_n|)$. This situation is approximately realized in the example considered before as shown in Fig. 3. We have checked in the same example that the sign of the energy difference plays no role. In other words, the same values of C and B can be used above and below E_n.

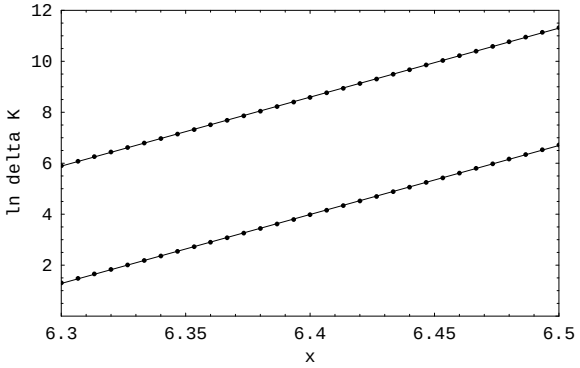

FIG. 3. Natural logarithm of $\delta K(x)$ for $E - E_0 = 10^{-30}$ (lower set of point) and $E - E_0 = 10^{-28}$ (upper set of point). Lines are linear fits.

The exponent B is not uniform. It increases with x and is $G-$dependent as shown in Fig. 4. The local values of B have been calculated by fits in regions of width 0.2 with central value displayed in the horizontal label of Fig. 4. In the coming Section, we show that it is possible to exploit the G-dependence in order to optimize the numerical treatment of the problem.

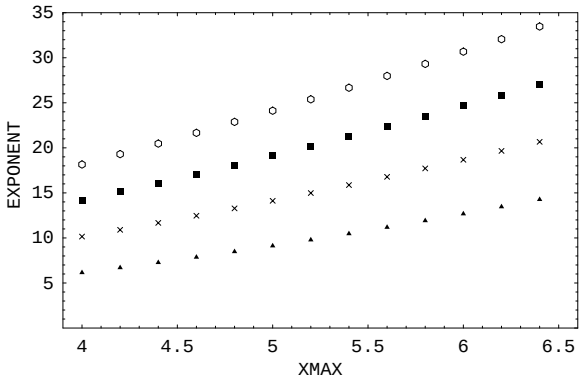

FIG. 4. Value of B for various x and for $G = -3x$ (empty hexagones), $G = -2x$ (filled squares) $G = -x$ (crosses) and $G = 0$ (triangles)

VII. AN OPTIMAL CHOICE OF G

In this Section, we consider again the calculation of the ground state in the case $m = 1/2$, $\hbar = 1, V_2 = 1$ and $V_4 = 0.1$. This case has been treated in the literature [18] and a numerical value with 30 digits is given in Ref. [10].

We shall estimate the ground state using the equation $K(x_{max}) = 0$ with $x_{max} = 6$. The fact that we use this finite value for x_{max} creates an error in the 25-th digit and it is not possible to go beyond this accuracy using that particular condition.

From the discussion of Section IV, it is reasonable to limit the discussion to a gauge function of the form

$$G(x) = -ax \ , \tag{15}$$

which using Eq. (7) implies that

$$K(x) \propto \Psi(x) \mathrm{e}^{\frac{1}{2\hbar}ax^2} \ . \tag{16}$$

With this restriction, the optimization problem is reduced to the determination of a. Eq. (16) also provides a simple intuitive interpretation of the results of Fig. 4: as a increases through positive values, the features of Ψ are exponentially amplified, making the bifurcation more violent. Ideally, we would like to take a as large as possible. However, if a is too large, we may need too many coefficients K_n to get a good approximation. If we consider the problem at a given order, the two requirements of sensitivity and accuracy result in a compromise which determines the optimal value of a.

As explained in Section IV, the choice of Eq. (15) guarantees a suppression of the form $(n!)^{\frac{-1}{3}}$ for the coefficients of L and K. However, the choice of a still affects significantly the behavior of these coefficients as shown in Fig. 5.

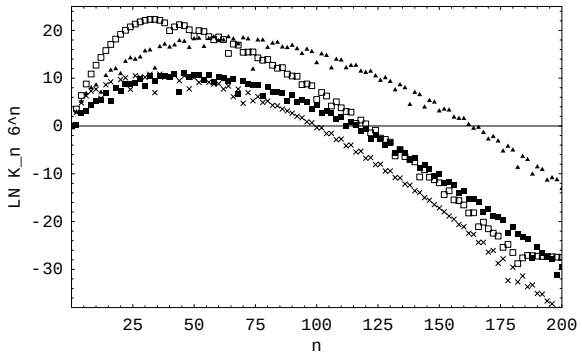

FIG. 5. $\ln(|K_n 6^n|)$ versus n, for $G = 0$ (triangles), $G = -x$ (filled squares), $G = -2x$ (crosses) and $G = -3x$ (empty squares).

The quantity $K_n x_{max}^n$ is relevant to decide at which order we need to truncate the series in order to get a good estimate of $K(x_{max})$. For instance, if we require to know $K(x_{max})$ with errors of order 1, we need about 100 coefficients for $a = 2$ but more than 150 for $a = 0$. The corresponding values for $a = 1$ and 3 fall between these two values, indicating that $a = 2$ is close to optimal. This estimate is confirmed by an analysis of the dependence of K_n on a. Sample values are shown in Fig. 6. We observe rapid oscillations (that we will not attempt to explain) and slowly varying amplitudes which have a minimum slightly below 2. Note that on the logarithmic scale of Fig. 6, the zeroes of K_n gives $-\infty$, however due to the discrete sampling of a, it just generates isolated dots on the graphs.

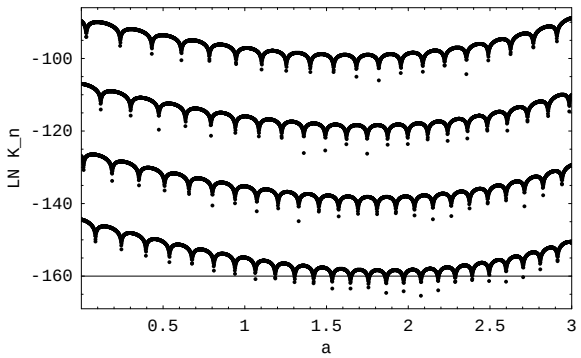

FIG. 6. $\ln(|K_n|)$ versus a, for n=60 (upper set), 70 (next set), 80 (next set) and 90 (lower set).

This point of view is further confirmed by considering the number of significant digits that can be obtained from the condition $K(6) = 0$ using an expansion of K truncated at a given order. From Fig. 7, we see for instance that for a truncation at order 100, the most accurate answer is obtained for $a \simeq 1.8$. It is worth noting that for this value of a, one gains more than 15 significant digits compared to the $G = 0$ case! This figure aslo indicates, that the best possible answer (in the present case, 25 significant digits) can always be achieved by calculating enough coefficients.

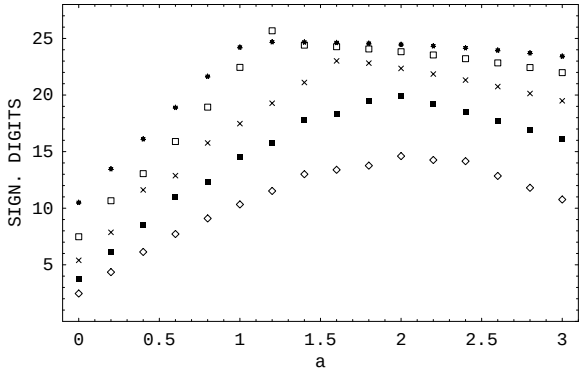

FIG. 7. Number of significant digits for E_0 versus a using the condition $K(6) = 0$ with expansions of order 50 (empty diamonds), 75 (filled squares), 100 (crosses), 125 (empty squares) and 150 (stars).

VIII. APPROXIMATE ERROR FORMULAS

The condition $K(x_{max}) = 0$ provides an exact solution of a modified problem where V becomes suddenly infinite at x_{max}. If $V(x_{max}) >> E_n$, one expects that the modified problem is very similar to the original one as far as the low energy spectrum is concerned. The large exponents found in Section V also indicate that the upper bound is very sharp. For completeness, we will in this

Section give a more quantitative discussion of the error as a function of x_{max} and the parameters appearing in the Hamiltonian. In this Section, we assume that V is parity invariant and we use the units $\hbar = m = 1$, $V_2 = 1/2$. The error for the harmonic oscillator has been estimated in Ref. [15]. The anharmonic corrections can be approximated by multiplying the error by a factor $\exp(-S_{anh})$, where

$$S_{anh} = \int_{-\infty}^{+\infty} dt V_{anh}(x_{max} \mathrm{e}^{-|t|}) \ , \tag{17}$$

and V_{anh} is the anharmonic part of the potential. The final estimate for the error on the ground state is

$$\delta E_0 \simeq 4\pi^{-1/2} x_{max}^2 \mathrm{e}^{-\sum_{j=2}^{l} (\frac{1}{j}) V_{2j} x_{max}^{2j}} \int_{x_{max}}^{+\infty} dx \mathrm{e}^{-x^2} \ . \tag{18}$$

We have tested this estimate for $V_{anh} = \lambda x^4$. The results are shown in Figs. 8 and 9. One sees that the estimate is good provided that λ is not too large.

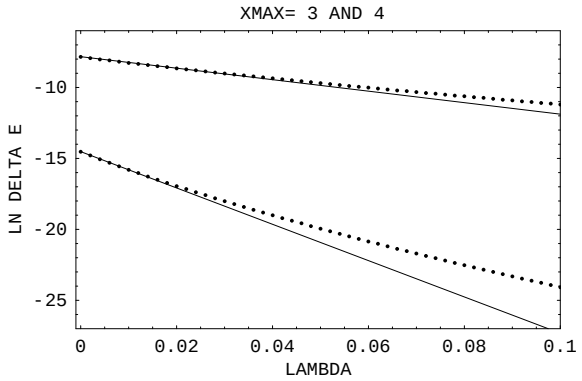

FIG. 8. $\ln(\delta E_0)$ as a function of λ for $x_{max} = 3$ (upper set of points) and x_{max}=4 (lower set of points). The continuous lines are drawn from Eq. (18).

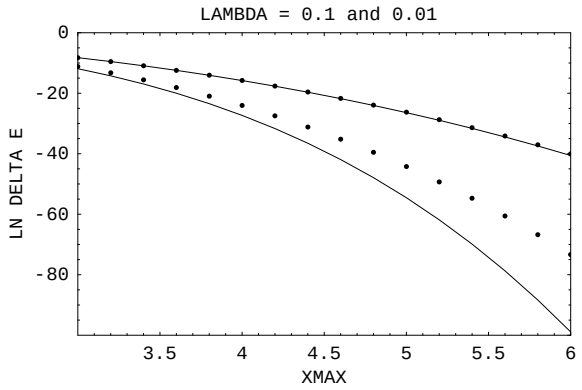

FIG. 9. $\ln(\delta E_0)$ as a function of x_{max} for $\lambda = 0.01$ (upper set of points) and λ=0.1 (lower set of points). The continuous lines are drawn from Eq. (18) .

IX. A CHALLENGING TEST

The only practical limitation of the method proposed here is that in some case the relevant details of the potential appear in widely separated regions, forcing us to calculate a huge number of coefficients with many significant digits. A simple example where such problem may occur is the symmetric double-well with a small quartic coupling where the separation between the wells goes like the inverse square root of the quartic coupling.

In Ref. [19], the lowest even and odd energies were calculated for a potential with $m = 1$, $\hbar = 1$, $V_2 = -1/4$, $V_4 = 1/2000$ with 180 significant digits. Remarkably, the authors were able to reproduce the 110 significant digits of the splitting between these two states by calculating instanton effects. We have reproduced the 180 digits of both states using an expansion of order 1700 for K and a value of $x_{max} = 46$. The calculations were performed with 700 digit arithmetic. The calculation of one level with such a procedure takes less than two hours with MATHEMATICA on an unexpensive laptop using Pentium3. The computation time increases with the accuracy required. In order to fix the ideas, it takes less than 2 minutes minutes to reproduce the first 120 digits in the above calculation.

X. CONCLUSIONS

In conclusion, we have shown that accurate estimates of the energy levels of arbitrary polynomial potentials bounded from below can be obtained by solving polynomial equations. The fact that the function L and K are entire guarantees that if we calculate enough terms we will gain proper control of the asymptotic behavior of the wave function. Reaching this goal is in general a difficult task which often requires guesswork and analytical continuations (see e.g., Ref. [20]). Here, the convergence of the procedure is guaranteed. In addition, a systematic understanding and control of the errors due to the finite value of x_{max} has been achieved.

The understanding of the gauge invariance of the basic equations proposed here completely resolves the issues raised from our initial proposal [10]. Spurious zeroes have disappeared and we reached an understanding of the mechanism responsible for the gauge optimization of the numerical calculation.

The extreme accuracy obtained for two widely separated wells indicates that for reasonably complicated potential, the number of terms that needs to be calculated is not prohibitive. We intend to use this method to test analytical results regarding the role of large configurations in the path-integral and to test semi-classical treatment of potentials with asymmetric wells [6,7].

ACKNOWLEDGMENTS

We thank B. Oktay for communicating his work regarding the treatment of parity non invariant potentials with the method of Ref. [10]. We thank P. Kleiber, W. Klink, L. Li, G. Payne, W. Polyzou, M.H. Reno and V.G.J. Rodgers for valuable conversations. This research was supported in part by the Department of Energy under Contract No. FG02-91ER40664, and in part by the CIFRE of the University of Iowa.

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